Variational Inference (Contd)

Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

Feb 13, 2019

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- A revision-cum-QA session on Friday (or Saturday?) 6:30pm in KD-101

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- Mean-field VI updates the q_j's in a cyclic manner, like ALT-OPT, Gibbs sampling, etc

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- Substituting the expressions $p(\mathbf{X}|\mu,\tau) = \prod_{n=1}^{N} p(x_n|\mu,\tau)$ and $\log p(\mu|\tau)$, we get

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- Proceeding in a similar way (verify), we can show that $q_\tau^*(\tau) = \text{Gamma}(\tau|a_N, b_N)$

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$$a_N = a_0 + \frac{N+1}{2} \quad \text{and} \quad b_N = b_0 + \frac{1}{2}\mathbb{E}_{q_\mu}\left[\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right]$$

Mean-Field VI: A Very Simple Example (Contd)

- Substituting the expressions $p(\mathbf{X}|\mu,\tau) = \prod_{n=1}^{N} p(x_n|\mu,\tau)$ and $\log p(\mu|\tau)$, we get

$$\begin{aligned}\log q_\mu^*(\mu) &= \mathbb{E}_{q_\tau}[\log p(\mathbf{X}|\mu,\tau) + \log p(\mu|\tau)] + \text{const} \\ &= -\frac{\mathbb{E}_{q_\tau}[\tau]}{2}\left\{\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right\} + \text{const}\end{aligned}$$

- (Verify) The above is log of a Gaussian. Thus $q_\mu^*(\mu) = \mathcal{N}(\mu|\mu_N,\tau_N)$ with

$$\mu_N = \frac{\lambda_0\mu_0 + N\bar{x}}{\lambda_0 + N} \quad \text{and} \quad \lambda_N = (\lambda_0 + N)\mathbb{E}_{q_\tau}[\tau]$$

- Proceeding in a similar way (verify), we can show that $q_\tau^*(\tau) = \text{Gamma}(\tau|a_N, b_N)$

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- Important: Updates of $q_\mu^*(\mu)$ and $q_\tau^*(\tau)$ depend on each-other (thus requires cyclic updates)

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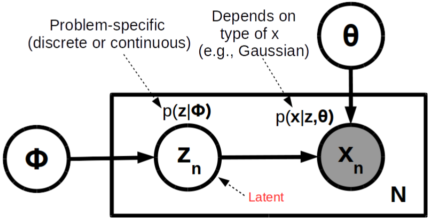
- Important/useful to keep these facts in mind (will use these later)

VI for Models with Local and Global Variables



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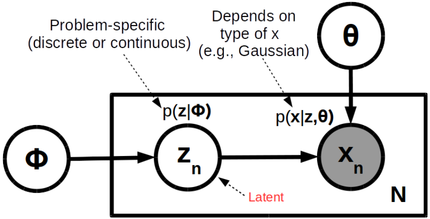

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  - GMM: $\mathbf{Z} = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N]$ are cluster ids, $\boldsymbol{\beta} = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \}_{k=1}^K$

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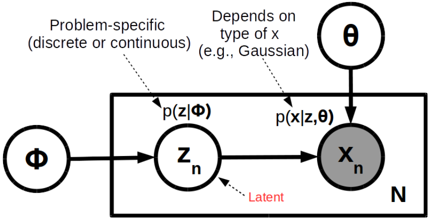

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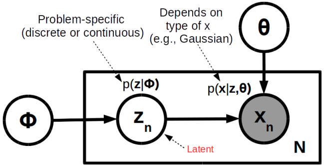
  - PPCA: $\mathbf{Z} = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N]$ are latent codes, $\boldsymbol{\beta}$ are params defining the "decoder" ($\boldsymbol{z}_n$ to $\boldsymbol{x}_n$ mapping)

VI for Models with Local and Global Variables (Contd)



- Assuming independence, the joint distribution of data $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ and unknowns $\mathbf{Z}, \beta$

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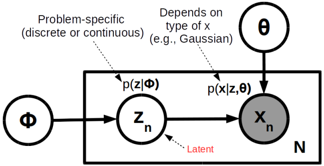

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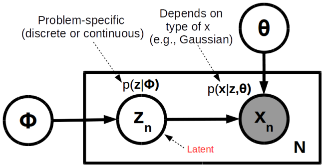

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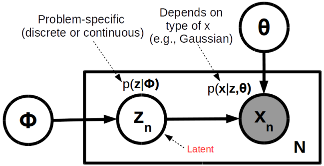

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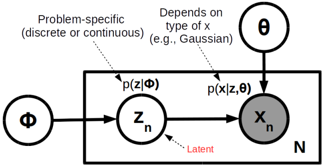

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where $\boldsymbol{\alpha} = [\alpha_1, \alpha_2]^\top$ are hyperparams of the prior $p(\boldsymbol{\beta})$ and $[\boldsymbol{\beta}, -A(\boldsymbol{\beta})]$ is the suff-stats vector

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- With the CPs for β and $\boldsymbol{z}_n$'s, deriving the mean-field VI updates for these is easy!

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- The mean-field VI updates will be as follows (PRML Sec 10.2)

$$\boxed{q^\star(\boldsymbol{\pi}) = \mathrm{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha})} \qquad \alpha_k = \alpha_0 + N_k$$

$$\boxed{q^\star(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) = \mathcal{N}\left(\boldsymbol{\mu}_k | \mathbf{m}_k, (\beta_k \boldsymbol{\Lambda}_k)^{-1}\right) \mathcal{W}(\boldsymbol{\Lambda}_k | \mathbf{W}_k, \nu_k)}$$

$$\begin{aligned}
\beta_k &= \beta_0 + N_k \\
\mathbf{m}_k &= \frac{1}{\beta_k}(\beta_0 \mathbf{m}_0 + N_k \overline{\mathbf{x}}_k) \\
\mathbf{W}_k^{-1} &= \mathbf{W}_0^{-1} + N_k \mathbf{S}_k + \frac{\beta_0 N_k}{\beta_0 + N_k}(\overline{\mathbf{x}}_k - \mathbf{m}_0)(\overline{\mathbf{x}}_k - \mathbf{m}_0)^{\mathrm{T}} \\
\nu_k &= \nu_0 + N_k.
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Posterior Predictive with VI Approximations

- Given a new observation $\hat{\boldsymbol{x}}$ and past data $\mathbf{X}$, the *true* posterior predictive for a GMM is

$$p(\widehat{\mathbf{x}}|\mathbf{X}) = \sum_{\widehat{\mathbf{z}}} \iiint p(\widehat{\mathbf{x}}|\widehat{\mathbf{z}}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) p(\widehat{\mathbf{z}}|\boldsymbol{\pi}) p(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}|\mathbf{X}) \, \mathrm{d}\boldsymbol{\pi} \, \mathrm{d}\boldsymbol{\mu} \, \mathrm{d}\boldsymbol{\Lambda}$$

$$p(\widehat{\mathbf{x}}|\mathbf{X}) = \sum_{k=1}^{K} \iiint \pi_k \mathcal{N}\left(\widehat{\mathbf{x}}|\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right) p(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}|\mathbf{X}) \, \mathrm{d}\boldsymbol{\pi} \, \mathrm{d}\boldsymbol{\mu} \, \mathrm{d}\boldsymbol{\Lambda}$$

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- Given the variational approx. of posterior, the posterior predictive can be approximated as

$$p(\widehat{\mathbf{x}}|\mathbf{X}) = \sum_{k=1}^{K} \iiint \pi_k \mathcal{N}\left(\widehat{\mathbf{x}}|\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right) q(\boldsymbol{\pi}) q(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) \, \mathrm{d}\boldsymbol{\pi} \, \mathrm{d}\boldsymbol{\mu}_k \, \mathrm{d}\boldsymbol{\Lambda}_k$$

$$p(\widehat{\mathbf{x}}|\mathbf{X}) = \frac{1}{\widehat{\alpha}} \sum_{k=1}^{K} \alpha_k \mathrm{St}(\widehat{\mathbf{x}}|\mathbf{m}_k, \mathbf{L}_k, \nu_k + 1 - D)$$

$$\mathbf{L}_k = \frac{(\nu_k + 1 - D)\beta_k}{(1 + \beta_k)} \mathbf{W}_k$$

Some Properties of VB

Recall that VB is equivalent to finding q by minimizing $\text{KL}(q||p)$

$$\text{KL}(q||p) = \int q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X})} \right]$$

If the true posterior $p(\mathbf{Z}|\mathbf{X})$ is very small in some region then, to minimize $\text{KL}(q||p)$, the approx. dist. q will also have to be very small (otherwise KL will be very large)

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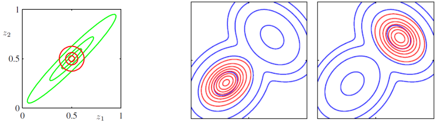
- Underestimates the variances of the true posterior
- For multimodal posteriors, VB locks onto one of the modes



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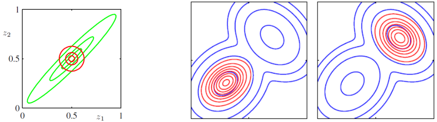

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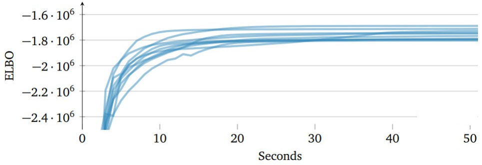
Note: Some other inference methods, e.g., Expectation Propagation (EP) can avoid this behavior

VI and Convergence

- VI is guaranteed to converge but only to a local optima (just like EM)
- Therefore proper initialization is important (just like EM)



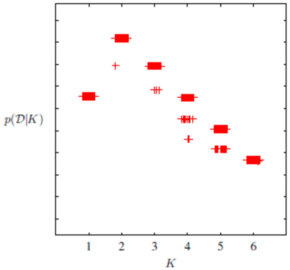
Different initializations may lead to different optima

- ELBO increases monotonically with iterations, so we can monitor the ELBO to assess convergence

ELBO for Model Selection

- Recall that ELBO is a lower bound on log of model evidence $\log p(\mathbf{X}|m)$)
- We can compute ELBO for each model m and then choose the one with largest value of ELBO
- An Example: The ELBO plot for a GMM with different K values (number of components)

Plot of the variational lower bound $\mathcal{L}$ versus the number K of components in the Gaussian mixture model, for the Old Faithful data, showing a distinct peak at $K = 2$ components. For each value of K, the model is trained from 100 different random starts, and the results shown as '$+$' symbols plotted with small random horizontal perturbations so that they can be distinguished. Note that some solutions find suboptimal local maxima, but that this happens infrequently.



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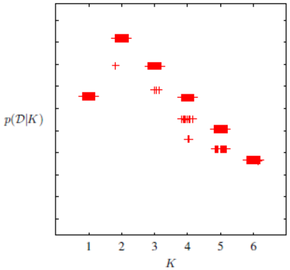

- Note that unlike likelihood, ELBO doesn't monotonically increase with K (penalizes large K)
- Some criticism since we are using a lower-bound but works well in practice in many problems

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- Since there is no notion of "parameters", VI is like EM without the "M step"

VI and Expectation Maximization (EM)

- VB can be seen as a generalization of the EM algorithm
- Unlike EM, in VI there is no distinction between parameters Θ and latent variables $\mathbf{Z}$
- VI treats all unknowns of the model as latent variables and calls them $\mathbf{Z}$
- Since there is no notion of "parameters", VI is like EM without the "M step"
- VI can be used within an EM algorithm if the E step is intractable
    - This is known as Variational EM algorithm

VI: The Road Ahead

- Moving beyond locally conjugate models
- Moving beyond the mean-field assumption
- More scalable variational inference
- General-purpose VI (that doesn't require model-specific derivations)
  - Posing VI as a general gradient based optimization problem

$$\phi^{new} = \phi^{old} + \eta \times \nabla_\phi \left[\mathbb{E}_{q_\phi}[\log p(\mathbf{X}, \mathbf{Z})] - \mathbb{E}_{q_\phi}[\log q(\mathbf{Z}|\phi)]\right]$$

  - A lot of recent research on approximating the gradient of an expectation
- We will look at these issues after mid-sem